PORTLAND HARBOR SUPERFUND SITE BIOACCUMULATION MODELING REPORT

APPENDIX C: MODEL DOCUMENTATION

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1.0 MODEL AND RATIONALE FOR CONVERSION TO VISUAL BASIC FOR APPLICATIONS

The primary goal of mechanistic modeling for the remedial investigation/feasibility study is to develop a predictive relationship between chemical concentrations in sediment, water, and tissue that can be used to derive preliminary sediment remediation goals and compare remedial alternatives for chemicals that are present in fish tissue, water, and sediment at concentrations associated with unacceptable risk. The mechanistic model used to calculate preliminary remediation goals (PRGs) in this report is based on algorithms and equations initially established by Gobas (1993). This model has been used as the basis for many subsequent updates and iterations of Gobas-type models, including refinements and simplifications (Arnot and Gobas 2004; Morrison et al. 1996, 1997). The driving force of these fugacity-based models is phase partitioning. The first type of partitioning occurs between water and the organism, and the second occurs during the digestion process between prey items or ingested sediment and the organism within the gastrointestinal tract.

Models based on the original Gobas (1993) approach have been used in a broad range of environments (i.e., lakes, rivers, and estuaries) as described in the 2004 technical memorandum on evaluating steady-state aquatic mechanistic models for the Portland Harbor Superfund site (Windward 2004). The model used for development of initial PRG (iPRGs) as presented in the Round 2 Comprehensive Report (Integral et al. 2007), and here for PRGs was adapted from the Arnot-Gobas (2004) model but was transferred into Visual Basic for Applications® (VBA) code. This conversion was primarily the work of Bruce Hope (senior environmental toxicologist with ODEQ) and was intended to increase the transparency of the model's function (EPA 2006; ODEQ 2006). The conversion to VBA code also served to reduce the effort required to enter parameters into the model. Section 3 provides a full presentation of the VBA code. The following description of the model is largely adapted from the VBA model description provided to LWG by Bruce Hope (ODEQ 2006).

Inputs and outputs for the VBA version of the mechanistic model are accomplished through the use of Microsoft® Excel® spreadsheets. An effort was made to avoid complicated (although perhaps more efficient) coding in order to preserve the transparency of the way the model functions (ODEQ 2006). Use of Excel® for the biotic model interface facilitates the concurrent use of Monte Carlo software (in this case, Crystal Ball®) for enhanced uncertainty and sensitivity analyses. This combination of software makes it possible to run multiple iterations of the model. This appendix describes the

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components of the model and then presents the VBA code used to run the model. The acronyms provided in the model and sub-model explanations (inputs and outputs) are the same as those used in the VBA code, unless otherwise indicated.

2.0 GENERAL PROCESSES AND STRUCTURE OF THE MODEL

The use of an overly detailed food web with numerous species categories would have exceeded both the availability of site-specific and literature-derived physiological data. The Lower Willamette River (LWR) mechanistic model working group, consisting of Lower Willamette Group (LWG) members and the US Environmental Protection Agency (EPA) and its partners, had several meetings and discussions to agree on the species to be modeled. Because the model's primary purpose is to inform remediation decisions and not to precisely predict tissue residues, a simplified food web was deemed sufficient (EPA 2006). Based on this premise, certain representative pelagic and benthic species were selected for modeling. The species groups that were modeled, and the representative species for which LWG data are available, are as follows:

- Phytoplankton
- Zooplankton
- Benthic invertebrate filter feeders (clams, *Corbicula fluminea*)
- Benthic invertebrate consumers ¹
- Epibenthic invertebrate consumers (crayfish, unidentified species)
- Foraging fish (sculpin, *Cottus* spp.)
- Benthivorous fish (largescale sucker, *Catostomus macrocheilus*)
- Omnivorous fish (common carp, *Cyprinus carpio*)
- Small piscivorous fish (smallmouth bass, *Micropterus dolomieui*)
- Large piscivorous fish (northern pikeminnow, *Ptychocheilus oregonensis*)

¹ A generalized category designed to represent oligochaetes, insect larvae, and amphipods.

2.1 MODEL SET-UP AND ASSUMPTIONS

The Arnot and Gobas mechanistic model that is the basis for this model was designed around the premise that a single equation may be used to represent the exchange of non-ionic organic chemicals between an organism and its environment (Arnot and Gobas 2004). The conceptual equation, which underlies the model and describes the net flux of a parent chemical being absorbed or deposited (dM_B) by an organism at any time (dt), is:

$$\frac{dM_B}{dt} = \left\{ W_B \cdot \left(k_1 \cdot \left[m_O \cdot C_{WD,O} + m_P C_{WD,P} \right] + k_D \cdot \sum_i \left(P_i \cdot C_{D,i} \right) \right) \right\} - \left(k_2 + k_E + k_M \right) \cdot M_B \qquad \text{Equation 1}$$

Where:

Acronym	Definition	Unit
M_{B}	Mass of chemical in organism	g
W_{B}	Wet weight of organism	kg
\mathbf{k}_1	Clearance rate constant for water ventilated by organism	L/kg×day
m_{O}	Fraction of respiratory ventilation involving overlying water	unitless
m_P	Fraction of respiratory ventilation involving porewater	unitless
$C_{WD,O}$	Total freely dissolved chemical concentration in overlying water	g/L
$C_{WD,P}$	Freely dissolved chemical concentration in porewater	g/L
k_D	Clearance rate constant via ingestion of food and water	kg/kg×day
$P_{\rm i}$	Fraction of the diet composed of prey item i	unitless
$C_{D,i}$	Chemical concentration in prey item i	g/kg
k_2	Gill and skin elimination rate constant	1/day
$k_{\rm E}$	Fecal egestion rate constant	1/day
K_{M}	Metabolic transformation rate constant	1/day

Because of a lack of adequate time-dependent data for the Portland Harbor Study Area, the model has been simplified to assume steady-state conditions for the purposes of this application. Therefore, per Arnot and Gobas (2004), the equation used to assess biomagnification and bioaccumulation up the food chain (and actually applied in the model) becomes:

$$C_{B} = \frac{k_{1} \times \left(m_{O} \times C_{WD,O} + m_{P} \times C_{WD,P}\right) + k_{D} \times \sum P_{i} \times C_{D,i}}{k_{2} + k_{E} + k_{G} + k_{M}}$$

Equation 2

Where:

Acronym	Definition	Unit
$C_{\rm B}$	Chemical concentration in biota tissue	g/kg ww
\mathbf{k}_1	Gill uptake rate constant	L/kg×day
m_o	Fraction of respiratory ventilation that involves overlying water	unitless
$C_{WD,O}$	Total freely dissolved chemical concentration in the water column above the sediment	g/L
m_p	Fraction of respiratory ventilation that involves sediment- associated porewater	unitless
$C_{\mathrm{WD,P}}$	Total freely dissolved chemical concentration in the sediment associated porewater	g/L
K_D	Dietary uptake rate constant	$kg/kg \times day$
\mathbf{P}_{i}	Fraction of the diet consisting of the prey item i	unitless
$C_{\mathrm{D,i}}$	Concentration of a chemical in a prey item	g/kg
\mathbf{k}_2	Gill elimination rate constant	1/day
$k_{\rm E}$	Fecal egestion rate constant	1/day
k_{G}	Growth rate constant	1/day
k_{M}	Metabolic transformation rate constant	1/day

A number of specific sub-models are used to define the rate coefficients and dissolved water concentrations in the steady-state equation. These submodels can be broken down into three categories: physical, chemical, and biological processes. Additional variables are required to parameterize the sub-models and are defined as below as the sub-models are presented.

2.2 PHYSICAL AND CHEMICAL PROCESSES

Inputs from physical site-specific data and literature were used to describe various physical processes required in the model to predict chemical flux through the environment. The following parameters were calculated by the model.

$$Z_{water} = \frac{1}{HT}$$
 Equation 3
$$Z_{lipid} = Z_{water} \times K_{OW}$$
 Equation 4
$$C_{ox} = (-0.24 T_w + 14.04) \times 0.9$$
 Equation 5

This document is currently under review by US EPA and its federal, state, and tribal partners, and is subject to change in whole or in part.

Where:

Acronym	Definition	Unit
Z_{water}	Water fugacity	mol m ⁻³ /Pa
Z_{lipid}	Lipid fugacity	mol m ^{-3/} Pa
HT	Temperature-compensated Henry's Law constant	Pa m ⁻³ /mol
K_{OW}	Chemical-specific octanol-water partition coefficient	kg/L
T_{w}	Mean water temperature	°C
C_{ox}	Dissolved oxygen content at 90% saturation	mg/L

Z_{lipid} is used in the calculation of chemical uptake from lipid and non-lipid organic matter (NLOM) in the gut during digestion. Zwater is used in the calculation of chemical uptake from water in the gut (see Section 2.3.3). C_{ox} is used to calculate the gill ventilation rate (Section 2.3.2).

Some of chemical and physical parameters were used to calculate bioavailable chemical concentrations in surface water (CwD o) and in porewater (C_{WD,P}). C_{WD,O} and C_{WD,P} were used to describe organism exposure through respiration.

In the Arnot and Gobas model (2004), the model calculates the fraction of dissolved and freely available chemical in the water column in the case that there is no available empirical data. The previous version of the model applied to the LWR (Windward 2005) estimated dissolved concentration from total water concentration. EPA and its partners recommended that the site-specific filtered surface water data (XAD column data) be used in future model iterations (EPA 2006). As in the Comprehensive Round 2 Report model (Integral et al. 2007), an equation was required to convert the site-specific filtered surface water data (XAD column data) to the dissolved concentration (C_{WD,O}) used in the model. The dissolved water concentration for chemicals was estimated using the following equation from Morrison et al. (1997).

$$C_{WD,O} = \frac{\text{filtered water concentration}}{1 + (K_{OW} \times 0.08 \times DOC)}$$
Equation 6

In Morrison et al. (1997), an adjustment was made (multiplying $0.5 \times$ dissolved organic carbon [DOC] in the denominator, not shown in the above equation) because the filter pore size used in the measurements for that study $(0.2 \mu m)$ was smaller than the diameter of DOC particles $(0.45 \mu m)$. The filter size for LWG DOC water sampling was 0.5 µm, so this adjustment was not necessary.

Because the model was modified to use XAD sample information, which directly estimates freely dissolved water concentration, no overlying water information (identified as previous versions on the model as ϕ or $C_{WT,O}$) (Arnot and Gobas 2004) was needed.

The concentration of a chemical freely dissolved in porewater (g/L), C_{WD,P}, can be estimated from the concentration of the chemical in sediment using the following equation.

$$C_{WD, P} = \frac{C_{S,OC}}{K_{OC}}$$
 Equation 7

In this equation, $C_{S,OC}$ (g/kg organic carbon) represents the concentration of the chemical in sediment after it has been normalized for organic carbon content. K_{OC} is the organic carbon-water partition coefficient (L/kg organic carbon).

2.3 GENERAL BIOLOGICAL PROCESSES

The general biological processes included in the model are described below. In some cases, the acronyms used by Arnot and Gobas (2004) and described below vary slightly from the acronyms used in the VBA model provided by Bruce Hope (ODEQ 2006). For example, the clearance rate via respiration is described below as k_1 and is included in the model code as K1, and the dietary absorption efficiency of lipid ε_L is included in the model code as eL.

2.3.1 Species Modeled and Dietary Apportionment

Aquatic food webs may be large and rather complex. At the recommendation of EPA and its partners (EPA 2006), the number of species included in the mechanistic model were reduced from the previous LWR mechanistic model (Windward 2005) and are the same as the version of the model presented in the Comprehensive Round 2 report (Integral et al. 2007). Through the LWR mechanistic model working group, a reduced number of trophic groups to be modeled and representative species for each group were agreed upon. For example, the "benthic invertebrate consumer" category was designed to represent oligochaetes, amphipods, and insect larvae. The dietary menu selected for the benthic invertebrate consumers trophic group was therefore designed to reflect the dietary preferences of all three of those species. Diets for each trophic group were then assigned by Windward Environmental LLC (Windward), incorporating comments from EPA and its partners (EPA 2006) and with consideration of all species that the trophic groups were intended to represent.

The selection of dietary prey items is fully discussed in Appendix D, which describes the selection of all parameters included in the model. Briefly, dietary compositions for fish and invertebrates were compiled primarily from studies in the LWR (ODFW 2005) and general qualitative observations of fish stomach contents collected during Round 1 sampling, as reported in Attachment B8 of Appendix B of the RI/FS Programmatic Work Plan (Integral et al. 2004). These stomach content analysis results were augmented with data from the general literature, including a study of dietary habits of Lower Columbia River fish (Zimmerman 1999).

Diets of fish and invertebrates are likely to be variable because of opportunistic feeding behavior and seasonal and spatial variations in prey availability. The presence of natural fluctuations in dietary preferences was addressed by normalizing dietary fractions across a "menu" of possible food items (as described in EPA 2006). This normalization was accomplished using a matrix spreadsheet provided by Bruce Hope (ODEQ 2006). When the model is run deterministically (a single iteration using point estimates), each trophic group is assigned one best estimate of dietary items and portion of each dietary item. When the model is run probabilistically (multiple model iterations using distributions), the portion of each dietary item consumed varies with each model iteration. The matrix ensures that the selected portions are normalized so the sum of dietary portion equals 1.

Dietary exposure to ingested prey tissue and ingested sediment affects the consumer during the digestion process. Phase partitioning occurs across the gut wall, and chemicals may be absorbed into the tissues or expelled from the tissues into the gut contents. This exchange of chemicals during the digestive process is discussed in greater detail in Section 2.3.3.

2.3.2 Direct Contact Through Water Exposure – Phase Partitioning

Organic chemicals are thought to partition between lipid, protein, and carbohydrate (collectively known as non-lipid organic matter [NLOM]), and water. The sorption and storage of chemicals may occur to a certain extent in each of these media for each organism modeled. Therefore, an organismwater partitioning coefficient (k_{BW}), which results from direct contact with water during respiration, is determined for each organism according to the following equation.

$$k_{BW} = \frac{k_1}{k_2} = VLB_{org} \times K_{OW} + VNB_{org} \times \beta \times K_{OW} + VWB_{org}$$
 Equation 8

Where:

Acronym	Definition	Unit
\mathbf{k}_1	Gill uptake rate constant	L/kg×day
\mathbf{k}_2	Gill elimination rate constant	d^{-1}
VLB_{org}	Lipid fraction of the organism	unitless
$\mathrm{VNB}_{\mathrm{org}}$	NLOM fraction of the organism	unitless
VWB_{org}	Water fraction of the organism	unitless
β (ВЕТА)	NLOM-octanol proportionality constant	unitless
K_{OW}	Chemical-specific octanol-water partition coefficient	kg/L

When calculating k_{BW} for phytoplankton, VNB_{org} is replaced by the NLOCoctanol proportionality constant (GAMMA). The constant GAMMA affects partitioning between water and non-lipid organic carbon (NLOC) (see Section 2.4.3).

In order to estimate the parameters k_1 and k_2 , Arnot and Gobas rely on the following set of sub-models (Arnot and Gobas 2004).

The gill uptake rate constant, k_1 , describes the rate at which chemicals are absorbed from water across the membranes of the gills and skin. It is considered a function of the ventilation rate (G_v, in units of L/day) and the diffusion rate across the surface, such that:

$$k_1 = \frac{E_W \times G_v}{W_B}$$
 Equation 9

Where:

= the chemical uptake efficiency across the gills as a percentage (%) W_{R} = the weight of the organism in kg

G_v is calculated as:

$$G_{V} = \frac{1,400 \times W_{B}^{0.65}}{C_{OX}}$$
 Equation 10

Where:

= the dissolved oxygen content (mg/L) = the weight of the organism in kg W_{B}

Arnot and Gobas (2004) propose a different method of calculating k_1 for algae and macrophytes. Instead of the equation presented above, the following relationship is recommended.

$$k_1 = [A + (B/K_{ow})]^{-1}$$
 Equation 11

In this equation, A and B are constants that represent the resistance of the algae or macrophytes to the uptake of the chemical through aqueous and organic phases, respectively. Based on empirical data described more fully in Arnot and Gobas (2004), default values of 6.0×10^{-5} and 5.5 were selected for constants A and B, respectively.

The gill elimination rate constant, k_2 , describes the rate at which chemicals are removed from the organism across the gill membrane. Closely related to k_1 , inasmuch as both constants are sensitive to ventilation rate and permeability across the surface of the gill membrane, k_2 is defined such that $k_2 = k_1/K_{\rm BW}$.

Because bioaccumulation is defined by the ratio of k_1 to k_2 , any errors that may occur in the selection of appropriate G_V and E_W values will be canceled out in the model. Therefore, the model is relatively insensitive to parameterization errors in G_V and E_W , which makes it possible to represent the ventilation rate and chemical uptake efficiency across the gill membrane with a single equation for a variety of species.

2.3.3 Direct Contact Through Dietary Exposure – Phase Partitioning

In addition to direct exposure to chemicals in the water, organisms may be exposed to chemicals present in ingested prey items.

The dietary uptake rate constant, k_D , defines the rate at which chemicals are removed from the gastrointestinal tract of an organism and absorbed into tissue. The dietary uptake rate constant is defined as $k_D = E_D \times G_D/W_B$, where E_D is the dietary chemical transfer efficiency, G_D is the feeding rate, and W_B is the weight of the organism. E_D has been shown to rely heavily on the K_{OW} value of the chemical being absorbed and therefore was defined by Arnot and Gobas (2004) based on a two-phase lipid-water resistance model. Thus, $E_D = (3.0 \times 10^{-7} \times K_{OW} + 2.0)^{-1}$. The first and last terms in this equation are defined as dietary uptake constants A and B, respectively (EDA and EDB). Feeding rates are best defined using site-specific empirical data, if such data are available. However, if such information does not exist for a particular site being modeled, feeding rate G_D may be defined as $G_D = 0.022 \times W_B^{0.85} \times \exp(0.06 \times T)$ for fish, zooplankton, and aquatic invertebrate species. In the absence of empirical data, the feeding rate of aquatic filter feeders is best

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defined as $G_D = G_V \times C_{SS} \times \sigma$, such that the feeding rate is a product of the gill ventilation rate (G_V) , the concentration of suspended solids $(C_{SS}$ in units of kg/L), and the scavenging efficiency of particles removed from water $(\sigma$ as a percentage, called in SCV in VBA model).

Chemicals may also be eliminated from an organism through fecal ingestion, which is defined by the fecal elimination rate constant k_E . This rate constant $k_E = G_F \times E_D \times K_{GB}/W_B$, where G_F is the fecal egestion rate, E_D is the dietary chemical transfer rate (described above), K_{GB} is the partitioning coefficient between the gut contents of the organism and its tissue, and W_B is the organism's weight. The fecal egestion rate G_F is a function of how digestible the various components of the diet are.

$$G_{F} = \{[(1-\varepsilon_{L}) \times V_{LD}] + [(1-\varepsilon_{N}) \times V_{ND}] + [(1-\varepsilon_{W}) \times V_{WD}] \} \times G_{D}.$$
 Equation 12

Where:

Acronym	Definition	Unit
$\epsilon_{ m L}$	Dietary assimilation efficiencies of lipid	unitless
$\epsilon_{ m N}$	Dietary assimilation efficiencies of NLOM	unitless
$\epsilon_{ m W}$	Dietary assimilation efficiencies of water	unitless
$ m V_{LD}$	Lipid fraction of the diet	unitless
$V_{ m ND}$	NLOM fraction of the diet	unitless
$ m V_{WD}$	Water fraction of the diet	unitless

It is estimated as $K_{GB} = (V_{LG} \times K_{OW} + V_{NG} \times \beta \times K_{OW} + V_{WG}) / (V_{LB} \times K_{OW} + V_{NB} \times \beta \times K_{OW} + V_{WB})$, where V_{LG} , V_{NG} , and V_{WG} are the lipid, NLOM, and water contents of the gut. These gut fractions are estimated as shown below; they collectively add up to a number approaching 1 and are dependent upon the assimilation efficiency fraction for each component. (Arnot and Gobas 2004) The fractions of lipid, NLOM, and water present in the tissue of the organism are described as V_{LB} , V_{NB} , and V_{WB} , respectively, and are based on organism-specific information.

$$V_{NG} = \frac{\left(\left[1 - \epsilon N \right] \times V_{LD} \right)}{\left(\left[1 - \epsilon L \right] \times V_{LD} \right) + \left(\left[1 - \epsilon N \right] \times V_{ND} \right) + \left(\left[1 - \epsilon W \right] \times V_{WD} \right)}$$
 Equation 14

$$V_{WG} = \frac{\left(\left[1 - \epsilon L \right] \times V_{WD} \right)}{\left(\left[1 - \epsilon L \right] \times V_{LD} \right) + \left(\left[1 - \epsilon N \right] \times V_{ND} \right) + \left(\left[1 - \epsilon W \right] \times V_{WD} \right)}$$
 Equation 15

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In the model, Z_{water} is used to determine chemical uptake from water in the gut (V_{WG}) , and Z_{lipid} is used to determine chemical uptake from both lipid matter in the gut (V_{LG}) and non-lipid organic matter in gut (V_{NG}) . These parameters are used in conjunction with the above equations to describe the chemical flux between an organism's tissue and the material in its gut (see Section 2.4.4 for full equation).

2.3.4 Growth

Growth rate information is available for a wide range of species. However, growth rates may vary between and within species according to a number of factors, including, but not limited to, the organism size and age, the environmental temperature, and the availability and quality of food (Arnot and Gobas 2004). The recommended approximation for growth rate in the absence of empirical data is $k_G = 0.0005 \times W_B^{-0.2}$ for temperatures around 10°C (Arnot and Gobas 2004; Thomann et al. 1992).

2.3.5 Metabolism

Chemical compounds may be eliminated from an organism through metabolic transformation, in which the parent compound undergoes structural changes to become a chemical derivative or metabolite of the original compound. The metabolic process is species- and chemical-specific, and the inclusion of metabolism in the mechanistic model is further discussed in Section 6.6 of Appendix D.

2.4 SPECIES-SPECIFIC CALCULATIONS

2.4.1 Overview

Many of the equations presented in Arnot and Gobas (2004) were included in the version of the model used in this food web modeling effort. Excerpts of the VBA code used to run the model for the LWR mechanistic model are presented below with explanations of each input parameter used and examples of how those parameters fit into the equations required to run the model. The parameter abbreviations used by Arnot and Gobas in the 2004 model were altered slightly for convenience in the version presented here (ODEQ 2006). However, the functionality of the model was preserved.

The entire VBA code is presented at the end of this section; but because of the iterative nature of the model, a representative organism from each of the three main types of organisms modeled (i.e., one plankton, one benthic invertebrate, and one fish) has been selected for a more detailed description

in this section. Section 3, the complete VBA code, presents the exact coding information used for the other organisms.

2.4.2 Identifying Numbers for Species Used in Equations

The identifying numbers used to represent species in the mechanistic model are presented in Table 1.

Table 1. Identifying Numbers for Species

Identifying Number	Species
2	Phytoplankton
3	Zooplankton
4	Clam
5	Worm (benthic invertebrate consumer)
6	Crayfish
7	Largescale sucker
8	Sculpin
9	Carp
10	Smallmouth bass
11	Northern pikeminnow

This numbering methodology allowed for the identification of speciesspecific values within the code without having to write out the entire species name as it accompanied each of the individual parameters.

2.4.3 Phytoplankton

VLB2 = empirical value defined by model user

VWB2 = empirical value defined by model user

VNB2 = 1-(VLB2 + VWB2)

K12 = 1/(UA + (UB/KOW))

KM2 = empirical data defined by user

KPW2 = (VLB2 * KOW) + (VNB2 * (GAMMA * 10) * KOW) + VWB2

K22 = K12/KPW2

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FPW2 = empirical data defined by user

$$CB2 = CWB * K12 * (1-FPW2)/(K2_2 + KG2 + KM2)$$

Acronym	Definition
VLB2	Lipid fraction of organism (unitless)
VNB2	Non-lipid organic matter fraction of organism (unitless)
VWB2	Water fraction of organism (unitless)
GAMMA	Non-lipid organic carbon (NLOC) proportionality constant (unitless)
K12	Gill uptake rate constant (d ⁻¹)
UA	Uptake constant A (unitless)
UB	Uptake constant B (unitless)
KOW	Chemical-specific octanol-water partition coefficient (kg/L)
KPW2	Organism-water partition coefficient (unitless)
K22	Gill elimination rate constant (d ⁻¹)
KG2	Growth rate constant (d ⁻¹)
KM2	Metabolic rate constant (d ⁻¹)
FPW2	Fraction of sediment porewater ventilated by organism (unitless)
CWB	Biologically available concentration of chemical in water (ng/g)
CB2	Predicted tissue concentration in organism (ng/g)

2.4.4 Benthic Invertebrate Filter Feeder (Clam)

WB4 = empirical value defined by user

VLB4 = empirical value defined by model user

VLBsed = empirical value defined by model user

VWB4 = empirical value defined by model user

VWBsed = empirical value defined by model user

VNB4 = 1-(VLB4 + VWB4)

VNBsed = empirical value defined by model user

WBL4 = WB4 * VLB4

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KM4 = empirical data defined by user

$$QW4 = 88.3 * WB4^{0.06}$$

$$QL4 = QW4 * 0.01$$

$$KG4 = 0.000502 * WB4^{-0.2}$$

$$GV4 = (1400 * (WB4^{0.065}))/COX$$

SCV4 = empirical value defined by model user

$$GD4 = GV4 * CPW * SCV4$$

DF4,1 = dietary fraction of prey item 1 (sediment) for organism 4 (clam)

DF4,2 = dietary fraction of prey item 2 (phytoplankton) for organism 4 (clam)

eL4 = empirical value defined by model user

eN4 = empirical value defined by model user

eW4 = empirical value defined by model user

FPW4 = empirical value defined by model user

Food
$$4A = DF4,2 * VLB2 + DF4,1 * VLBsed$$

Food
$$4B = DF4,2 * VNB2 + DF4,1 * VNBsed$$

Food
$$4C = DF4,2 * VWB2 + DF4,1 * VWBsed$$

Food
$$4D = DF4,2 * CB2 + DF4,1 * CST$$

$$GF4 = (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C))) * GD4$$

$$VLG4 = ((1 - eL4) * Food4A) / (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C))$$

$$VNG4 = ((1 - eN4) * Food4B) / (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C))$$

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$$VWG_4 = ((1 - eW4) * Food4C) / (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C))$$

$$ED4 = 1 / (EDA * KOW + EDB)$$

$$KD4 = ED4 * GD4 / WB4$$

$$EWW4 = 1 / (1.89 + (155 / KOW))$$

$$K14 = 1/((UA + (UB/KOW)))$$

$$K24 = K14/KPW4$$

FPW4 = empirical data defined by model user

$$KGB4 = Zgut4 / Zorg4$$

$$KE4 = KGB4 / WB4 * ED4 * GF4$$

Definition
Lipid fraction of organism (unitless)
Non-lipid organic matter fraction of organism (unitless)
Water fraction of organism (unitless)
Lipid fraction of organism (unitless); always equal to 0
Organic carbon content of sediment
Water fraction of sediment (unitless); always equal to 0
Filter feeder scavenging efficiency
Organism body weight (kg)
Organism lipid weight (kg)
Aqueous transport parameter for organism (d-1)
Lipid transport parameter for organism (d-1)
Food ingestion rate (kg food/day)

DO NOT QUOTE OR CITE

Acronym	Definition
TW	Mean water temperature (°C)
KG4	Growth rate constant (d-1)
GV4	Gill ventilation rate (L d-1)
COX	Dissolved oxygen content at 90% saturation (mg/L)
CPW	Concentration of suspended solids (kg/L)
DF4,2	Fraction of phytoplankton in invertebrate diet (unitless)
DF4,3	Fraction of zooplankton in invertebrate diet (unitless)
DF4,1	Fraction of sediment in invertebrate diet (unitless)
FoodA4	Intermediate calculation term (unitless)
FoodB4	Intermediate calculation term (unitless)
FoodC4	Intermediate calculation term (unitless)
FoodD4	Intermediate calculation term (unitless)
GF4	Fecal egestion rate (kg food/day)
eL4	Lipid dietary absorption efficiency for organism (unitless)
eN4	NLOM dietary absorption efficiency for organism (unitless)
eW4	Water dietary absorption efficiency for organism (unitless)
VLG4	Lipid fraction in organism gut (unitless)
VNG4	NLOM fraction in organism gut (unitless)
VWG4	Water fraction in organism gut (unitless)
ED4	Intestinal tract chemical transfer efficiency (unitless)
EDA	Dietary chemical transfer constant A
EDB	Dietary chemical transfer constant B
KD4	Dietary uptake rate constant (d-1)
K14	Gill uptake rate constant (d-1)
EWW4	Gill chemical transfer efficiency (unitless)
UA	Uptake constant A (unitless)
UB	Uptake constant B (unitless)
KOW	Chemical-specific octanol-water partition coefficient (kg/L)
KPW4	Organism-water partition coefficient (unitless)
K24	Gill elimination rate constant (d ⁻¹)
BETA	NLOM proportionality constant (unitless)
Zorg4	Organism fugacity (mol m ⁻³ Pa ⁻¹)
Zgut4	Organism intestinal tract fugacity (mol m ⁻³ Pa ⁻¹)
Zlipid	Lipid fugacity
Zwater	Water fugacity
KGB4	Gut-organism partition coefficient (unitless)
KE4	Fecal egestion rate constant (d ⁻¹)
KM4	Metabolic rate constant (d ⁻¹)
FPW4	Fraction of sediment porewater ventilated (unitless)
CWD	Biologically available concentration of chemical in water (ng/g)
CST	Total concentration of chemical in sediment (ng/g)
CSD	Concentration of chemical in sediment porewater (ng/g)
CB4	Tissue concentration in organism (ng/g)

2.4.5 Fish (Sculpin)

WB7 = empirical value defined by model user

VLB7 = empirical value defined by model user

VWB7 = empirical value defined by model user

VNB7 = 1 - (VLB7 + VWB7)

WBL7 = WB7 * VLB7

KM7 = empirical value defined by model user

 $QW7 = 88.3 * WB7^{0.6}$

QL7 = QW7 * 0.01

 $KG7 = 0.000502 * WB7^{-0.2}$

 $GV7 = (1400 * (WB7^{0.65})) / COX$

 $GD7 = 0.022 * WB7^{0.85} * Exp(0.06 * T_W)$

DF71 = dietary fraction of prey item 1 (sediment) for organism 7 (sculpin)

DF72 = dietary fraction of prey item 2 (phytoplankton) for organism 7 (sculpin)

DF73 = dietary fraction of prey item 3 (zooplankton for) organism 7 (sculpin)

DF74 = dietary fraction of prey item 4 (clam) for organism 7 (sculpin)

DF75 = dietary fraction of prey item 5 (worm) for organism 7 (sculpin)

DF76 = dietary fraction of prey item 6 (crayfish) for organism 7 (sculpin)

eL7 = empirical value defined by model user

eN7 = empirical value defined by model user

eW7 = empirical value defined by model user

FPW7 = empirical value defined by model user

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$$GF7 = (((1 - eL7) * Food7A) + ((1 - eN7) * Food7B) + ((1 - eW7) * Food7C)) * GD7$$

$$VLG7 = ((1 - eL7) * Food7A) / (((1 - eL7) * Food7A) + ((1 - eN7) * Food7B) + ((1 - eW7) * Food7C))$$

$$VNG7 = ((1 - eN7) * Food7B) / (((1 - eL7) * Food7A) + ((1 - eN7) * Food7B) + ((1 - eW7) * Food7C))$$

$$VWG7 = ((1 - eW7) * Food7C) / (((1 - eL7) * Food7A) + ((1 - eN7) * Food7B) + ((1 - eW7) * Food7C))$$

$$ED7 = 1 / (EDA * KOW + EDB)$$

$$KD7 = ED7 * GD7 / WB7$$

$$EWW7 = 1 / (1.89 + (155 / KOW))$$

$$K17 = EWW7 * GV7 / WB7$$

$$KPW7 = (VLB7 * KOW) + (VNB7 * BETA * KOW) + VWB7$$

$$K27 = K17 / KPW7$$

$$KGB7 = Zgut7 / Zorg7$$

$$KE7 = KGB7 / WB7 * ED7 * GF7$$

$$CB7 = (CWB * K17 * (1 - FPW7) + CSD * K17 * FPW7 + KD7 * FoodD7) / (K27 + KE7 + KG7 + KM7)$$

Acronym	Definition
VLB7	Lipid fraction of organism (unitless)
VNB7	Non-lipid organic matter fraction of organism (unitless)
VWB7	Water fraction of organism (unitless)
WB7	Organism body weight (kg)
WBL7	Organism lipid weight (kg)
QW7	Aqueous transport parameter for organism (d ⁻¹)
QL7	Lipid transport parameter for organism (d ⁻¹)
GD7	Food ingestion rate (kg food/day)
TW	Mean water temperature (°C)
KG7	Growth rate constant (d ⁻¹)
GV7	Gill ventilation rate (L/day)
COX	Dissolved oxygen content at 90% saturation (mg/L)
DF	Fraction of other organism in fish diet (unitless).
FoodA7	Intermediate calculation term (unitless)
FoodB7	Intermediate calculation term (unitless)
FoodC7	Intermediate calculation term (unitless)
FoodD7	Intermediate calculation term (unitless)
VLBsed	Lipid fraction of organism (unitless); always equal to 0
VNBsed	Organic carbon content of sediment
VWBsed	Water content of sediment(unitless); always equal to 0
GF7	Fecal egestion rate (kg food/day)
eL7	Lipid dietary absorption efficiency for organism (unitless)
eN7	NLOM dietary absorption efficiency for organism (unitless)
eW7	Water dietary absorption efficiency for organism (unitless)
VLG7	Lipid fraction in organism gut (unitless)
VNG7	NLOM fraction in organism gut (unitless)
VWG7	Water fraction in organism gut (unitless)
ED7	Intestinal tract chemical transfer efficiency (unitless)
KD7	Dietary uptake rate constant (d ⁻¹)
EDA	Dietary chemical transfer constant A
EDB	Dietary chemical transfer constant B
K17	Gill uptake rate constant (d ⁻¹)
EWW7	Gill chemical transfer efficiency (unitless)
KOW	Chemical-specific octanol-water partition coefficient (kg/L)
KPW7	Organism-water partition coefficient (unitless)
K27	Gill elimination rate constant (d ⁻¹)
BETA	NLOM proportionality constant (unitless)
Zorg7	Organism fugacity (mol m ⁻³ Pa ⁻¹)
Zgut7	Organism intestinal tract fugacity (mol m ⁻³ Pa ⁻¹)

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Acronym	Definition
Zlipid	Lipid fugacity
Zwater	Water fugacity
KGB7	Gut-organism partition coefficient (unitless)
KE7	Fecal egestion rate constant (d ⁻¹)
KM7	Metabolic rate constant (d ⁻¹)
FPW7	Fraction of sediment porewater ventilated (unitless)
CWB	Biologically available concentration of chemical in water (ng/g)
CST	Total concentration of chemical in sediment (ng/g)
CSD	Concentration of chemical in sediment porewater (ng/g)
CB7	Tissue concentration in 7th organism (ng/g)

3.0 COMPLETE VBA CODE

Option Base 1

'___

Dim DT As Single

Dim KOW As Single

Dim BETA As Single

Dim GAMMA As Single

Dim EDA As Single

Dim EDB As Single

Dim HT As Single

Dim TW As Single

Dim CPW As Single

Dim CWB As Single

Dim CST As Single

Dim CSD As Single

Dim FPW2 As Single

Dim FPW3 As Single

Dim FPW4 As Single

Dim FPW5 As Single

Dim FPW6 As Single

Dim FPW7 As Single

Dim FPW8 As Single

Dim FPW9 As Single

Dim Zwater As Single

Dim Zlipid As Single

Dim VLBsed As Single

Dim VNBsed As Single

Dim VWBsed As Single

Dim COX As Single

Dim H As Single

Dim CWT As Single

Dim XPOC As Single

Dim APOC As Single

Dim DPOC As Single

Dim ADOC As Single

Dim BSF As Single

'___

Dim WB2 As Single

Dim VLB2 As Single

Dim VNB2 As Single

Dim VWB2 As Single

Dim UA As Single

Dim UB As Single

Dim K12 As Single

Dim K22 As Single

Dim KPW2 As Single

Dim KG2 As Single

Dim CB2 As Single

'____

Dim WB3 As Single

Dim VLB3 As Single

Dim VNB3 As Single

Dim VWB3 As Single

Dim WBL3 As Single

Dim KM3 As Single

Dim QW3 As Single

Dim QL3 As Single

Dim GD3 As Single

Dim KG3 As Single

Dim GV3 As Single

Dim DF32 As Single

Dim eL3 As Single

Dim eN3 As Single

Dim eW3 As Single

Dim GF3 As Single

Dim VLG3 As Single

Dim VNG3 As Single

Dim VWG3 As Single

Dim ED3 As Single

Dim KD3 As Single

Dim EWW3 As Single

Dim K13 As Single

Dim KPW3 As Single

Dim K23 As Single

Dim KE3 As Single

Dim Food3A As Single

Dim Food3B As Single

Dim Food3C As Single

Dim Zorg3 As Single

Dim Zgut3 As Single

Dim KGB3 As Single

Dim CB3 As Single

'____

Dim WB4 As Single

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Dim VLB4 As Single

Dim VNB4 As Single

Dim VWB4 As Single

Dim WBL4 As Single

Dim KM4 As Single

Dim QW4 As Single

Dim QL4 As Single

Dim GD4 As Single

Dim KG4 As Single

Dim GV4 As Single

Dim DF41 As Single

Dim DF42 As Single

Dim DF43 As Single

Dim eL4 As Single

Dim eN4 As Single

Dim eW4 As Single

Dim GF4 As Single

Dim VLG4 As Single

Dim VNG4 As Single

Dim VWG4 As Single

Dim ED4 As Single

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Dim KD4 As Single

Dim EWW4 As Single

Dim K14 As Single

Dim KPW4 As Single

Dim K24 As Single

Dim KE4 As Single

Dim SCV4 As Single

Dim Food4A As Single

Dim Food4B As Single

Dim Food4C As Single

Dim Food4D As Single

Dim Zorg4 As Single

Dim Zgut4 As Single

Dim KGB4 As Single

Dim CB4 As Single

•____

Dim WB5 As Single

Dim VLB5 As Single

Dim VNB5 As Single

Dim VWB5 As Single

Dim WBL5 As Single

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Dim KM5 As Single

Dim QW5 As Single

Dim QL5 As Single

Dim GD5 As Single

Dim KG5 As Single

Dim GV5 As Single

Dim DF51 As Single

Dim DF52 As Single

Dim DF53 As Single

Dim DF54 As Single

Dim eL5 As Single

Dim eN5 As Single

Dim eW5 As Single

Dim GF5 As Single

Dim VLG5 As Single

Dim VNG5 As Single

Dim VWG5 As Single

Dim ED5 As Single

Dim KD5 As Single

Dim EWW5 As Single

Dim K15 As Single

Dim GD6 As Single

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Dim KPW5 As Single Dim K25 As Single Dim KE5 As Single Dim Food5A As Single Dim Food5B As Single Dim Food5C As Single Dim Food5D As Single Dim Zorg5 As Single Dim Zgut5 As Single Dim KGB5 As Single Dim CB5 As Single Dim WB6 As Single Dim VLB6 As Single Dim VNB6 As Single Dim VWB6 As Single Dim WBL6 As Single Dim KM6 As Single Dim QW6 As Single Dim QL6 As Single

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Dim KG6 As Single

Dim GV6 As Single

Dim DF61 As Single

Dim DF62 As Single

Dim DF63 As Single

Dim DF64 As Single

Dim DF65 As Single

Dim eL6 As Single

Dim eN6 As Single

Dim eW6 As Single

Dim GF6 As Single

Dim VLG6 As Single

Dim VNG6 As Single

Dim VWG6 As Single

Dim ED6 As Single

Dim KD6 As Single

Dim EWW6 As Single

Dim K16 As Single

Dim KPW6 As Single

Dim K26 As Single

Dim KE6 As Single

Dim DF71 As Single

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Dim Food6A As Single Dim Food6B As Single Dim Food6C As Single Dim Food6D As Single Dim Zorg6 As Single Dim Zgut6 As Single Dim KGB6 As Single Dim CB6 As Single Dim WB7 As Single Dim VLB7 As Single Dim VNB7 As Single Dim VWB7 As Single Dim WBL7 As Single Dim KM7 As Single Dim QW7 As Single Dim QL7 As Single Dim GD7 As Single Dim KG7 As Single Dim GV7 As Single

Dim DF72 As Single

Dim DF73 As Single

Dim DF74 As Single

Dim DF75 As Single

Dim DF76 As Single

Dim eL7 As Single

Dim eN7 As Single

Dim eW7 As Single

Dim GF7 As Single

Dim VLG7 As Single

Dim VNG7 As Single

Dim VWG7 As Single

Dim ED7 As Single

Dim KD7 As Single

Dim EWW7 As Single

Dim K17 As Single

Dim KPW7 As Single

Dim K27 As Single

Dim KE7 As Single

Dim Food7A As Single

Dim Food7B As Single

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Dim KG8 As Single

Dim GV8 As Single

Dim DF81 As Single

Dim DF82 As Single

Dim DF83 As Single

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Dim Food7C As Single Dim Food7D As Single Dim Zorg7 As Single Dim Zgut7 As Single Dim KGB7 As Single Dim CB7 As Single Dim WB8 As Single Dim VLB8 As Single Dim VNB8 As Single Dim VWB8 As Single Dim WBL8 As Single Dim KM8 As Single Dim QW8 As Single Dim QL8 As Single Dim GD8 As Single

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Dim DF84 As Single

Dim DF85 As Single

Dim DF86 As Single

Dim DF87 As Single

Dim eL8 As Single

Dim eN8 As Single

Dim eW8 As Single

Dim GF8 As Single

Dim VLG8 As Single

Dim VNG8 As Single

Dim VWG8 As Single

Dim ED8 As Single

Dim KD8 As Single

Dim EWW8 As Single

Dim K18 As Single

Dim KPW8 As Single

Dim K28 As Single

Dim KE8 As Single

Dim Food8A As Single

Dim Food8B As Single

Dim Food8C As Single

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Dim Food8D As Single Dim Zorg8 As Single Dim Zgut8 As Single

Dim KGB8 As Single

Dim CB8 As Single

Dim WB9 As Single

Dim VLB9 As Single

Dim VNB9 As Single

Dim VWB9 As Single

Dim WBL9 As Single

Dim KM9 As Single

Dim QW9 As Single

Dim QL9 As Single

Dim GD9 As Single

Dim KG9 As Single

Dim GV9 As Single

Dim DF91 As Single

Dim DF92 As Single

Dim DF93 As Single

Dim DF94 As Single

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Dim DF95 As Single

Dim DF96 As Single

Dim DF97 As Single

Dim DF98 As Single

Dim eL9 As Single

Dim eN9 As Single

Dim eW9 As Single

Dim GF9 As Single

Dim VLG9 As Single

Dim VNG9 As Single

Dim VWG9 As Single

Dim ED9 As Single

Dim KD9 As Single

Dim EWW9 As Single

Dim K19 As Single

Dim KPW9 As Single

Dim K29 As Single

Dim KE9 As Single

Dim Food9A As Single

Dim Food9B As Single

Dim Food9C As Single

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Dim Food9D As Single

Dim Zorg9 As Single

Dim Zgut9 As Single

Dim KGB9 As Single

Dim CB9 As Single

'____

Dim WB10 As Single

Dim VLB10 As Single

Dim VNB10 As Single

Dim VWB10 As Single

Dim WBL10 As Single

Dim KM10 As Single

Dim QW10 As Single

Dim QL10 As Single

Dim GD10 As Single

Dim KG10 As Single

Dim GV10 As Single

Dim DF101 As Single

Dim DF102 As Single

Dim DF103 As Single

Dim DF104 As Single

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Dim DF105 As Single

Dim DF106 As Single

Dim DF107 As Single

Dim DF108 As Single

Dim DF109 As Single

Dim eL10 As Single

Dim eN10 As Single

Dim eW10 As Single

Dim GF10 As Single

Dim VLG10 As Single

Dim VNG10 As Single

Dim VWG10 As Single

Dim ED10 As Single

Dim KD10 As Single

Dim EWW10 As Single

Dim K110 As Single

Dim KPW10 As Single

Dim K210 As Single

Dim KE10 As Single

Dim FPW10 As Single

Dim Food10A As Single

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Dim Food10B As Single

Dim Food10C As Single

Dim Food10D As Single

Dim Zorg10 As Single

Dim Zgut10 As Single

Dim KGB10 As Single

Dim CB10 As Single

Dim WB11 As Single

Dim VLB11 As Single

Dim VNB11 As Single

Dim VWB11 As Single

Dim WBL11 As Single

Dim KM11 As Single

Dim QW11 As Single

Dim QL11 As Single

Dim GD11 As Single

Dim KG11 As Single

Dim GV11 As Single

Dim DF111 As Single

Dim DF112 As Single

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Dim DF113 As Single

Dim DF114 As Single

Dim DF115 As Single

Dim DF116 As Single

Dim DF117 As Single

Dim DF118 As Single

Dim DF119 As Single

Dim DF1110 As Single

Dim eL11 As Single

Dim eN11 As Single

Dim eW11 As Single

Dim GF11 As Single

Dim VLG11 As Single

Dim VNG11 As Single

Dim VWG11 As Single

Dim ED11 As Single

Dim KD11 As Single

Dim EWW11 As Single

Dim K111 As Single

Dim KPW11 As Single

Dim K211 As Single

Dim KE11 As Single

Dim FPW11 As Single

Dim Food11A As Single

Dim Food11B As Single

Dim Food11C As Single

Dim Food11D As Single

Dim Zorg11 As Single

Dim Zgut11 As Single

Dim KGB11 As Single

Dim CB11 As Single

Private dic As Scripting. Dictionary

'Private Const PHYTOPLANKTON As String = "phytoplankton"

Private Const ZOOPLANKTON As String = "zooplankton"

Private Const BI_FILTER_FEEDER As String = "benthic filter feeder"

Private Const BI_CONSUMER As String = "benthic consumer"

Private Const EBI_CONSUMER As String = "epibenthic consumer"

Private Const SCULPIN As String = "sculpin"

Private Const LARGESCALE_SUCKER As String = "largescale sucker"

Private Const CARP As String = "carp"

Private Const SMALLMOUTH_BASS As String = "smallmouth bass"

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Private Const NORTHERN PIKEMINNOW As String = "northern pikeminnow"

Public Function TissueConcentration(species As String, r As Range) As Single

PHFWPRG5

TissueConcentration = CSng(dic.Item(species))

End Function

Sub PHFWPRG5()

Set dic = New Scripting.Dictionary

'INPUT COMMON BIOLOGICAL PARAMETERS

KOW = 10 ^ Worksheets("inputs").Cells(4, 4)

VLBsed = 0

VNBsed = Worksheets("inputs").Cells(5, 4) 'same as OCSS

VWBsed = 1 - VNBsed

EDA = Worksheets("inputs").Cells(25, 4)

EDB = Worksheets("inputs").Cells(26, 4)

BETA = Worksheets("inputs").Cells(27, 4)

GAMMA = Worksheets("inputs").Cells(28, 4)

INPUT PHYSICOCHEMICAL & CONCENTRATION PARAMETERS

H = Worksheets("inputs").Cells(6, 4)

TW = Worksheets("inputs").Cells(7, 4)

Zwater = 1 / HT

Zlipid = Zwater * KOW

COX = (-0.24 * TW + 14.04) * 0.9

CPW = Worksheets("inputs").Cells(8, 4)

CWT = Worksheets("inputs").Cells(9, 4)

XPOC = Worksheets("inputs").Cells(16, 4)

APOC = Worksheets("inputs").Cells(17, 4)

DPOC = Worksheets("inputs").Cells(18, 4)

ADOC = Worksheets("inputs").Cells(19, 4)

BSF = 1 / (1 + (XPOC * APOC * KOW + DPOC * ADOC * KOW))

CWB = Worksheets("inputs").Cells(10, 4)

CST = Worksheets("inputs").Cells(11, 4)

CSD = Worksheets("inputs").Cells(12, 4)

'PHYTOPLANKTON (2)

VLB2 = Worksheets("inputs").Cells(32, 5)

VWB2 = Worksheets("inputs").Cells(33, 5)

VNB2 = 1 - (VLB2 + VWB2)

UA = Worksheets("inputs").Cells(23, 4)

UB = Worksheets("inputs").Cells(24, 4)

K12 = 1 / (UA + (UB / KOW))

KPW2 = (VLB2 * KOW) + (VNB2 * GAMMA * KOW) + VWB2

K22 = K12 / KPW2

KG2 = Worksheets("inputs").Cells(41, 5)

FPW2 = Worksheets("inputs").Cells(37, 5)

CB2 = (CWB * K12 * (1 - FPW2)) / (K22 + KG2)

dic.Add PHYTOPLANKTON, CB2

'ZOOPLANKTON (3)

WB3 = Worksheets("inputs").Cells(31, 6)

VLB3 = Worksheets("inputs").Cells(32, 6)

VWB3 = Worksheets("inputs").Cells(33, 6)

VNB3 = 1 - (VLB3 + VWB3)

WBL3 = WB3 * VLB3

KM3 = Worksheets("inputs").Cells(42, 6)

 $QW3 = 88.3 * WB3 ^ 0.6$

QL3 = QW3 * 0.01

 $GD3 = 0.022 * WB3 ^ 0.85 * Exp(0.06 * TW)$

 $KG3 = 0.000502 * WB3 ^ -0.2$

 $GV3 = (1400 * (WB3 ^ 0.65)) / COX$

DF32 = Worksheets("DF").Cells(4, 3)

eL3 = Worksheets("inputs").Cells(34, 6)

eN3 = Worksheets("inputs").Cells(35, 6)

eW3 = Worksheets("inputs").Cells(36, 6)

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Food3A = DF32 * VLB2

Food3B = DF32 * VNB2

Food3C = DF32 * VWB2

$$GF3 = (((1 - eL3) * Food3A) + ((1 - eN3) * Food3B) + ((1 - eW3) * Food3C)) * GD3$$

$$VLG3 = ((1 - eL3) * Food3A) / (((1 - eL3) * Food3A) + ((1 - eN3) * Food3B) + ((1 - eW3) * Food3C))$$

$$VNG3 = ((1 - eN3) * Food3B) / (((1 - eL3) * Food3A) + ((1 - eN3) * Food3B) + ((1 - eW3) * Food3C))$$

$$VWG3 = ((1 - eW3) * Food3C) / (((1 - eL3) * Food3A) + ((1 - eN3) * Food3B) + ((1 - eW3) * Food3C))$$

ED3 = 1 / (EDA * KOW + EDB)

KD3 = ED3 * GD3 / WB3

EWW3 = 1 / (1.89 + (155 / KOW))

K13 = EWW3 * GV3 / WB3

$$KPW3 = (VLB3 * KOW) + (VNB3 * BETA * KOW) + VWB3$$

K23 = K13 / KPW3

KGB3 = Zgut3 / Zorg3

KE3 = KGB3 / WB3 * ED3 * GF3

FPW3 = Worksheets("inputs").Cells(37, 6)

$$CB3 = (CWB * K13 * (1 - FPW3) + CB2 * KD3 * DF32) / (K23 + KE3 + KG3 + KM3)$$

dic.Add ZOOPLANKTON, CB3

'BENTHIC INVERTEBRATE - FILTER FEEDER (4)

$$VNB4 = 1 - (VLB4 + VWB4)$$

$$WBL4 = WB4 * VLB4$$

$$QW4 = 88.3 * WB4 ^ 0.6$$

$$QL4 = QW4 * 0.01$$

$$KG4 = 0.000502 * WB4 ^ -0.2$$

$$GV4 = (1400 * (WB4 ^ 0.65)) / COX$$

$$GD4 = GV4 * CPW * SCV4$$

$$DF42 = Worksheets("DF").Cells(5, 3)$$

$$Food4A = DF42 * VLB2 + DF41 * VLBsed$$

$$Food4B = DF42 * VNB2 + DF41 * VNBsed$$

$$Food4D = DF42 * CB2 + DF41 * CST$$

$$GF4 = (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C)) * GD4$$

$$VLG4 = ((1 - eL4) * Food4A) / (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C))$$

$$VNG4 = ((1 - eN4) * Food4B) / (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C))$$

$$VWG4 = ((1 - eW4) * Food4C) / (((1 - eL4) * Food4A) + ((1 - eN4) * Food4B) + ((1 - eW4) * Food4C))$$

$$ED4 = 1 / (EDA * KOW + EDB)$$

$$KD4 = ED4 * GD4 / WB4$$

$$EWW4 = 1 / (1.89 + (155 / KOW))$$

$$K14 = EWW4 * GV4 / WB4$$

$$KPW4 = (VLB4 * KOW) + (VNB4 * BETA * KOW) + VWB4$$

$$K24 = K14 / KPW4$$

$$KGB4 = Zgut4 / Zorg4$$

$$KE4 = KGB4 / WB4 * ED4 * GF4$$

dic.Add BI_FILTER_FEEDER, CB4

'BENTHIC INVERTEBRATE (CONSUMER) (5)

WB5 = Worksheets("inputs").Cells(31, 8)

VLB5 = Worksheets("inputs").Cells(32, 8)

VWB5 = Worksheets("inputs").Cells(33, 8)

VNB5 = 1 - (VLB5 + VWB5)

WBL5 = WB5 * VLB5

KM5 = Worksheets("inputs").Cells(42, 8)

 $QW5 = 88.3 * WB5 ^ 0.6$

QL5 = QW5 * 0.01

 $KG5 = 0.000502 * WB5 ^ -0.2$

 $GV5 = (1400 * (WB5 ^ 0.65)) / COX$

 $GD5 = 0.022 * WB5 ^ 0.85 * Exp(0.06 * TW)$

DF51 = Worksheets("DF").Cells(6, 2)

DF52 = Worksheets("DF").Cells(6, 3)

DF53 = Worksheets("DF").Cells(6, 4)

DF54 = Worksheets("DF").Cells(6, 5)

eL5 = Worksheets("inputs").Cells(34, 8)

eN5 = Worksheets("inputs").Cells(35, 8)

eW5 = Worksheets("inputs").Cells(36, 8)

FPW5 = Worksheets("inputs").Cells(37, 8)

Food5A = DF51 * VLBsed + DF52 * VLB2 + DF53 * VLB3 + DF54 * VLB4

Food5B = DF51 * VNBsed + DF52 * VNB2 + DF53 * VNB3 + DF54 * VNB4

$$GF5 = (((1 - eL5) * Food5A) + ((1 - eN5) * Food5B) + ((1 - eW5) * Food5C)) * GD5$$

$$VLG5 = ((1 - eL5) * Food5A) / (((1 - eL5) * Food5A) + ((1 - eN5) * Food5B) + ((1 - eW5) * Food5C))$$

$$VNG5 = ((1 - eN5) * Food5B) / (((1 - eL5) * Food5A) + ((1 - eN5) * Food5B) + ((1 - eW5) * Food5C))$$

$$VWG5 = ((1 - eV5) * Food5C) / (((1 - eL5) * Food5A) + ((1 - eV5) * Food5B) + ((1 - eV5) * Food5C))$$

$$ED5 = 1 / (EDA * KOW + EDB)$$

$$KD5 = ED5 * GD5 / WB5$$

$$EWW5 = 1 / (1.89 + (155 / KOW))$$

$$K15 = EWW5 * GV5 / WB5$$

$$KPW5 = (VLB5 * KOW) + (VNB5 * BETA * KOW) + VWB5$$

$$K25 = K15 / KPW5$$

$$KGB5 = Zgut5 / Zorg5$$

$$KE5 = KGB5 / WB5 * ED5 * GF5$$

dic.Add BI_CONSUMER, CB5

'EPIBENTHIC INVERTEBRATE (CONSUMER) (6)

WB6 = Worksheets("inputs").Cells(31, 9)

VLB6 = Worksheets("inputs").Cells(32, 9)

VWB6 = Worksheets("inputs").Cells(33, 9)

VNB6 = 1 - (VLB6 + VWB6)

WBL6 = WB6 * VLB6

KM6 = Worksheets("inputs").Cells(42, 9)

 $QW6 = 88.3 * WB6 ^ 0.6$

QL6 = QW6 * 0.01

 $KG6 = 0.000502 * WB6 ^ -0.2$

 $GV6 = (1400 * (WB6 ^ 0.65)) / COX$

 $GD6 = 0.022 * WB6 ^ 0.85 * Exp(0.06 * TW)$

DF61 = Worksheets("DF").Cells(7, 2)

DF62 = Worksheets("DF").Cells(7, 3)

DF63 = Worksheets("DF").Cells(7, 4)

DF64 = Worksheets("DF").Cells(7, 5)

DF65 = Worksheets("DF").Cells(7, 6)

eL6 = Worksheets("inputs").Cells(34, 9)

eN6 = Worksheets("inputs").Cells(35, 9)

eW6 = Worksheets("inputs").Cells(36, 9)

FPW6 = Worksheets("inputs").Cells(37, 9)

Food6A = DF61 * VLBsed + DF62 * VLB2 + DF63 * VLB3 + DF64 * VLB4 + DF65 * VLB5

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$$GF6 = (((1 - eL6) * Food6A) + ((1 - eN6) * Food6B) + ((1 - eW6) * Food6C)) * GD6$$

$$VLG6 = ((1 - eL6) * Food6A) / (((1 - eL6) * Food6A) + ((1 - eN6) * Food6B) + ((1 - eW6) * Food6C))$$

$$VNG6 = ((1 - eN6) * Food6B) / (((1 - eL6) * Food6A) + ((1 - eN6) * Food6B) + ((1 - eW6) * Food6C))$$

$$VWG6 = ((1 - eV6) * Food6C) / (((1 - eL6) * Food6A) + ((1 - eV6) * Food6B) + ((1 - eV6) * Food6C))$$

$$ED6 = 1 / (EDA * KOW + EDB)$$

$$KD6 = ED6 * GD6 / WB6$$

$$EWW6 = 1 / (1.89 + (155 / KOW))$$

$$K16 = EWW6 * GV6 / WB6$$

$$KPW6 = (VLB6 * KOW) + (VNB6 * BETA * KOW) + VWB6$$

$$K26 = K16 / KPW6$$

$$KE6 = KGB6 / WB6 * ED6 * GF6$$

$$CB6 = (CWB * K16 * (1 - FPW6) + CSD * K16 * FPW6 + KD6 * Food6D) / (K26 + KE6 + KG6 + KM6)$$

dic.Add EBI_CONSUMER, CB6

$$VNB7 = 1 - (VLB7 + VWB7)$$

$$WBL7 = WB7 * VLB7$$

$$QW7 = 88.3 * WB7 ^ 0.6$$

$$QL7 = QW7 * 0.01$$

$$KG7 = 0.000502 * WB7 ^ -0.2$$

$$GV7 = (1400 * (WB7 ^ 0.65)) / COX$$

$$GD7 = 0.022 * WB7 ^ 0.85 * Exp(0.06 * TW)$$

eW7 = Worksheets("inputs").Cells(36, 10)

FPW7 = Worksheets("inputs").Cells(37, 10)

Food7A = DF71 * VLBsed + DF72 * VLB2 + DF73 * VLB3 + DF74 * VLB4 + DF75 * VLB5 + DF76 * VLB6

Food7B = DF71 * VNBsed + DF72 * VNB2 + DF73 * VNB3 + DF74 * VNB4 + DF75 * VNB5 + DF76 * VNB6

Food7C = DF71 * VWBsed + DF72 * VWB2 + DF73 * VWB3 + DF74 * VWB4 + DF75 * VWB5 + DF76 * VWB6

Food7D = DF71 * CST + DF72 * CB2 + DF73 * CB3 + DF74 * CB4 + DF75 * CB5 + DF76 * CB6

GF7 = (((1 - eL7) * Food7A) + ((1 - eN7) * Food7B) + ((1 - eW7) * Food7C)) * GD7

VLG7 = ((1 - eL7) * Food7A) / (((1 - eL7) * Food7A) + ((1 - eN7) * Food7B) + ((1 - eN7) *eW7) * Food7C))

VNG7 = ((1 - eN7) * Food7B) / (((1 - eL7) * Food7A) + ((1 - eN7) * Food7B) + ((1 - eN7) *eW7) * Food7C)

VWG7 = ((1 - eV7) * Food7C) / (((1 - eL7) * Food7A) + ((1 - eV7) * Food7B) + ((1 - eV7) *eW7) * Food7C))

ED7 = 1 / (EDA * KOW + EDB)

KD7 = ED7 * GD7 / WB7

EWW7 = 1 / (1.89 + (155 / KOW))

K17 = EWW7 * GV7 / WB7

KPW7 = (VLB7 * KOW) + (VNB7 * BETA * KOW) + VWB7

K27 = K17 / KPW7

Zorg7 = (VLB7 * Zlipid) + (VNB7 * BETA * Zlipid) + (VWB7 * Zwater)

Zgut7 = VLG7 * Zlipid + VNG7 * BETA * Zlipid + VWG7 * Zwater

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'DF82 = Worksheets("DF").Cells(8, 3)

'DF83 = Worksheets("DF").Cells(8, 4)

'DF84 = Worksheets("DF").Cells(8, 5)

'DF85 = Worksheets("DF").Cells(8, 6)

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DF81 = Worksheets("DF").Cells(9, 2)

DF82 = Worksheets("DF").Cells(9, 3)

DF83 = Worksheets("DF").Cells(9, 4)

DF84 = Worksheets("DF").Cells(9, 5)

DF85 = Worksheets("DF").Cells(9, 6)

DF86 = Worksheets("DF").Cells(9, 7)

DF87 = Worksheets("DF").Cells(9, 8)

eL8 = Worksheets("inputs").Cells(34, 11)

eN8 = Worksheets("inputs").Cells(35, 11)

eW8 = Worksheets("inputs").Cells(36, 11)

FPW8 = Worksheets("inputs").Cells(37, 11)

Food8A = DF81 * VLBsed + DF82 * VLB2 + DF83 * VLB3 + DF84 * VLB4 + DF85 * VLB5 + DF86 * VLB6 + DF87 * VLB7

Food8B = DF81 * VNBsed + DF82 * VNB2 + DF83 * VNB3 + DF84 * VNB4 + DF85 * VNB5 + DF86 * VNB6 + DF87 * VNB7

Food8C = DF81 * VWBsed + DF82 * VWB2 + DF83 * VWB3 + DF84 * VWB4 + DF85 * VWB5 + DF86 * VWB6 + DF87 * VWB7

Food8D = DF81 * CST + DF82 * CB2 + DF83 * CB3 + DF84 * CB4 + DF85 * CB5 + DF86 * CB6 + DF87 * CB7

GF8 = (((1 - eL8) * Food8A) + ((1 - eN8) * Food8B) + ((1 - eW8) * Food8C)) * GD8

VLG8 = ((1 - eL8) * Food8A) / (((1 - eL8) * Food8A) + ((1 - eN8) * Food8B) + ((1 - eW8) * Food8C))

VNG8 = ((1 - eN8) * Food8B) / (((1 - eL8) * Food8A) + ((1 - eN8) * Food8B) + ((1 - eN8) * Food8C))

$$VWG8 = ((1 - eW8) * Food8C) / (((1 - eL8) * Food8A) + ((1 - eN8) * Food8B) + ((1 - eW8) * Food8C))$$

$$ED8 = 1 / (EDA * KOW + EDB)$$

$$KD8 = ED8 * GD8 / WB8$$

$$EWW8 = 1 / (1.89 + (155 / KOW))$$

$$K18 = EWW8 * GV8 / WB8$$

$$KPW8 = (VLB8 * KOW) + (VNB8 * BETA * KOW) + VWB8$$

$$K28 = K18 / KPW8$$

$$KGB8 = Zgut8 / Zorg8$$

$$KE8 = KGB8 / WB8 * ED8 * GF8$$

dic.Add LARGESCALE_SUCKER, CB8

'CARP - OMNIVORE (9)

$$VNB9 = 1 - (VLB9 + VWB9)$$

$$WBL9 = WB9 * VLB9$$

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$$QW9 = 88.3 * WB9 ^ 0.6$$

$$QL9 = QW9 * 0.01$$

$$KG9 = 0.000502 * WB9 ^ -0.2$$

$$GV9 = (1400 * (WB9 ^ 0.65)) / COX$$

$$GD9 = 0.022 * WB9 ^ 0.85 * Exp(0.06 * TW)$$

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$$GF9 = (((1 - eL9) * Food9A) + ((1 - eN9) * Food9B) + ((1 - eW9) * Food9C)) * GD9$$

$$VLG9 = ((1 - eL9) * Food9A) / (((1 - eL9) * Food9A) + ((1 - eN9) * Food9B) + ((1 - eW9) * Food9C))$$

$$VNG9 = ((1 - eN9) * Food9B) / (((1 - eL9) * Food9A) + ((1 - eN9) * Food9B) + ((1 - eW9) * Food9C))$$

$$VWG9 = ((1 - eW9) * Food9C) / (((1 - eL9) * Food9A) + ((1 - eN9) * Food9B) + ((1 - eW9) * Food9C))$$

$$ED9 = 1 / (EDA * KOW + EDB)$$

$$KD9 = ED9 * GD9 / WB9$$

$$EWW9 = 1 / (1.89 + (155 / KOW))$$

$$K19 = EWW9 * GV9 / WB9$$

$$KPW9 = (VLB9 * KOW) + (VNB9 * BETA * KOW) + VWB9$$

$$K29 = K19 / KPW9$$

$$KGB9 = Zgut9 / Zorg9$$

$$KE9 = KGB9 / WB9 * ED9 * GF9$$

dic.Add CARP, CB9

'SMALLMOUTH BASS - SMALL PISCIVORE (10)

$$VNB10 = 1 - (VLB10 + VWB10)$$

$$WBL10 = WB10 * VLB10$$

$$QW10 = 88.3 * WB10 ^ 0.6$$

$$QL10 = QW10 * 0.01$$

$$KG10 = 0.000502 * WB10 ^ -0.2$$

$$GV10 = (1400 * (WB10 ^ 0.65)) / COX$$

$$GD10 = 0.022 * WB10 ^ 0.85 * Exp(0.06 * TW)$$

$$DF101 = Worksheets("DF").Cells(11, 2)$$

$$DF104 = Worksheets("DF").Cells(11, 5)$$

$$DF105 = Worksheets("DF").Cells(11, 6)$$

$$DF106 = Worksheets("DF").Cells(11, 7)$$

$$DF108 = Worksheets("DF").Cells(11, 9)$$

$$DF109 = Worksheets("DF").Cells(11, 10)$$

eL10 = Worksheets("inputs").Cells(34, 13)

eN10 = Worksheets("inputs").Cells(35, 13)

eW10 = Worksheets("inputs").Cells(36, 13)

FPW10 = Worksheets("inputs").Cells(37, 13)

Food10A = DF101 * VLBsed + DF102 * VLB2 + DF103 * VLB3 + DF104 * VLB4 + DF105 * VLB5 + DF106 * VLB6 + DF107 * VLB7 + DF108 * VLB8 + DF109 * VLB9

Food10B = DF101 * VNBsed + DF102 * VNB2 + DF103 * VNB3 + DF104 * VNB4 + DF105 * VNB5 + DF106 * VNB6 + DF107 * VNB7 + DF108 * VNB8 + DF109 * VNB9

Food10C = DF101 * VWBsed + DF102 * VWB2 + DF103 * VWB3 + DF104 * VWB4 + DF105 * VWB5 + DF106 * VWB6 + DF107 * VWB7 + DF108 * VWB8 + DF109 * VWB9

Food10D = DF101 * CST + DF102 * CB2 + DF103 * CB3 + DF104 * CB4 + DF105 * CB5 + DF106 * CB6 + DF107 * CB7 + DF108 * CB8 + DF109 * CB9

GF10 = (((1 - eL10) * Food10A) + ((1 - eN10) * Food10B) + ((1 - eW10) * Food10C)) *GD10

VLG10 = ((1 - eL10) * Food10A) / (((1 - eL10) * Food10A) + ((1 - eN10) * Food10B) + ((1 - eN10((1 - eW10) * Food10C))

VNG10 = ((1 - eN10) * Food10B) / (((1 - eL10) * Food10A) + ((1 - eN10) * Food10B) + ((1 - eN10((1 - eW10) * Food10C))

VWG10 = ((1 - eV10) * Food10C) / (((1 - eL10) * Food10A) + ((1 - eV10) * Food10B)+ ((1 - eW10) * Food10C))

ED10 = 1 / (EDA * KOW + EDB)

KD10 = ED10 * GD10 / WB10

EWW10 = 1 / (1.89 + (155 / KOW))

K110 = EWW10 * GV10 / WB10

KPW10 = (VLB10 * KOW) + (VNB10 * BETA * KOW) + VWB10

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This document is currently under review by US EPA and its federal, state, and tribal partners, and is subject to change in whole or in part.

$$K210 = K110 / KPW10$$

$$KGB10 = Zgut10 / Zorg10$$

$$KE10 = KGB10 / WB10 * ED10 * GF10$$

$$CB10 = (CWB * K110 * (1 - FPW10) + CSD * K110 * FPW10 + KD10 * Food10D) / (K210 + KE10 + KG10 + KM10)$$

dic.Add SMALLMOUTH BASS, CB10

'NORTHERN PIKEMINNOW - LARGE PISCIVORE (11)

$$VNB11 = 1 - (VLB11 + VWB11)$$

$$QL11 = QW11 * 0.01$$

$$KG11 = 0.000502 * WB11 ^ -0.2$$

$$GV11 = (1400 * (WB11 ^ 0.65)) / COX$$

$$GD11 = 0.022 * WB11 ^ 0.85 * Exp(0.06 * TW)$$

$$DF112 = Worksheets("DF").Cells(12, 3)$$

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DF114 = Worksheets("DF").Cells(12, 5)
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$$DF115 = Worksheets("DF").Cells(12, 6)$$

$$DF116 = Worksheets("DF").Cells(12, 7)$$

$$DF119 = Worksheets("DF").Cells(12, 10)$$

$$DF1110 = Worksheets("DF").Cells(12, 11)$$

$$GF11 = (((1 - eL11) * Food11A) + ((1 - eN11) * Food11B) + ((1 - eW11) * Food11C)) * GD11$$

$$VLG11 = ((1 - eL11) * Food11A) / (((1 - eL11) * Food11A) + ((1 - eN11) * Food11B) + ((1 - eW11) * Food11C))$$

DO NOT QUOTE OR CITE

$$VNG11 = ((1 - eN11) * Food11B) / (((1 - eL11) * Food11A) + ((1 - eN11) * Food11B) + ((1 - eW11) * Food11C))$$

$$VWG11 = ((1 - eW11) * Food11C) / (((1 - eL11) * Food11A) + ((1 - eN11) * Food11B) + ((1 - eW11) * Food11C))$$

ED11 = 1 / (EDA * KOW + EDB)

KD11 = ED11 * GD11 / WB11

EWW11 = 1 / (1.89 + (155 / KOW))

K111 = EWW11 * GV11 / WB11

KPW11 = (VLB11 * KOW) + (VNB11 * BETA * KOW) + VWB11

K211 = K111 / KPW11

Zorg11 = (VLB11 * Zlipid) + (VNB11 * BETA * Zlipid) + (VWB11 * Zwater)

Zgut11 = VLG11 * Zlipid + VNG11 * BETA * Zlipid + VWG11 * Zwater

KGB11 = Zgut11 / Zorg11

KE11 = KGB11 / WB11 * ED11 * GF11

CB11 = (CWB * K111 * (1 - FPW11) + CSD * K111 * FPW11 + KD11 * Food11D) / (K211 + KE11 + KG11 + KM11)

dic.Add NORTHERN_PIKEMINNOW, CB11

End Sub

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